



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2023 – 02:31 AM EDT

PDB ID : 3W9G
Title : Crystal structure of the ankyrin repeat domain of chicken TRPV4
Authors : Itoh, Y.; Hamada-nakahara, S.; Suetsugu, S.
Deposited on : 2013-04-04
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

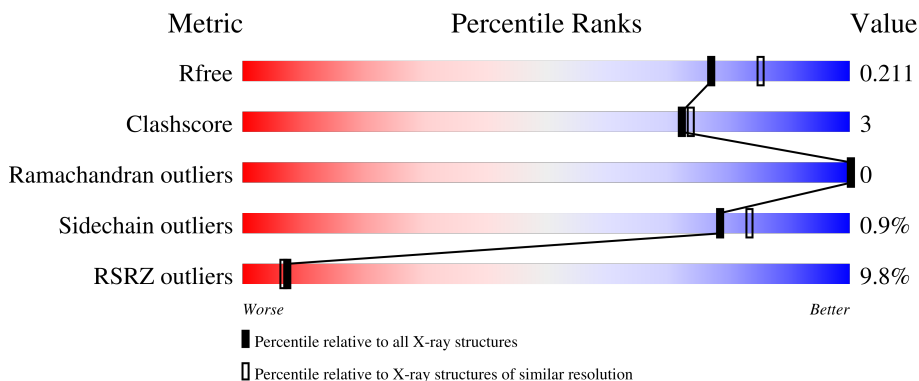
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

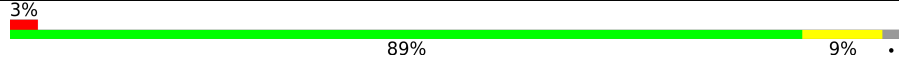
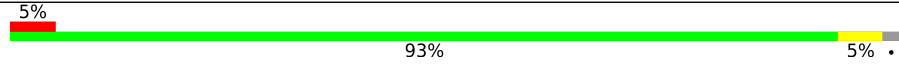
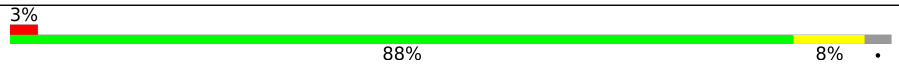

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	 3% 89% 9%
1	B	260	 5% 93% 5%
1	C	260	 3% 88% 8%
1	D	260	 27% 80% 17%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 8741 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Vanilloid receptor-related osmotically activated channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	Total	C	N	O	S	0	6	0
			2065	1307	382	367	9			
1	B	256	Total	C	N	O	S	0	5	0
			2058	1302	379	368	9			
1	C	252	Total	C	N	O	S	0	3	0
			2009	1273	366	361	9			
1	D	252	Total	C	N	O	S	0	0	0
			2001	1267	366	360	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	expression tag	UNP Q9DFS3
A	383	ALA	-	expression tag	UNP Q9DFS3
A	384	ALA	-	expression tag	UNP Q9DFS3
A	385	ALA	-	expression tag	UNP Q9DFS3
A	386	HIS	-	expression tag	UNP Q9DFS3
A	387	HIS	-	expression tag	UNP Q9DFS3
A	388	HIS	-	expression tag	UNP Q9DFS3
A	389	HIS	-	expression tag	UNP Q9DFS3
A	390	HIS	-	expression tag	UNP Q9DFS3
A	391	HIS	-	expression tag	UNP Q9DFS3
B	132	MET	-	expression tag	UNP Q9DFS3
B	383	ALA	-	expression tag	UNP Q9DFS3
B	384	ALA	-	expression tag	UNP Q9DFS3
B	385	ALA	-	expression tag	UNP Q9DFS3
B	386	HIS	-	expression tag	UNP Q9DFS3
B	387	HIS	-	expression tag	UNP Q9DFS3
B	388	HIS	-	expression tag	UNP Q9DFS3
B	389	HIS	-	expression tag	UNP Q9DFS3
B	390	HIS	-	expression tag	UNP Q9DFS3
B	391	HIS	-	expression tag	UNP Q9DFS3
C	132	MET	-	expression tag	UNP Q9DFS3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	383	ALA	-	expression tag	UNP Q9DFS3
C	384	ALA	-	expression tag	UNP Q9DFS3
C	385	ALA	-	expression tag	UNP Q9DFS3
C	386	HIS	-	expression tag	UNP Q9DFS3
C	387	HIS	-	expression tag	UNP Q9DFS3
C	388	HIS	-	expression tag	UNP Q9DFS3
C	389	HIS	-	expression tag	UNP Q9DFS3
C	390	HIS	-	expression tag	UNP Q9DFS3
C	391	HIS	-	expression tag	UNP Q9DFS3
D	132	MET	-	expression tag	UNP Q9DFS3
D	383	ALA	-	expression tag	UNP Q9DFS3
D	384	ALA	-	expression tag	UNP Q9DFS3
D	385	ALA	-	expression tag	UNP Q9DFS3
D	386	HIS	-	expression tag	UNP Q9DFS3
D	387	HIS	-	expression tag	UNP Q9DFS3
D	388	HIS	-	expression tag	UNP Q9DFS3
D	389	HIS	-	expression tag	UNP Q9DFS3
D	390	HIS	-	expression tag	UNP Q9DFS3
D	391	HIS	-	expression tag	UNP Q9DFS3

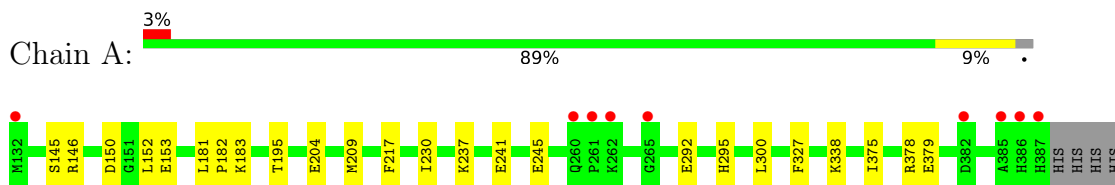
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	205	Total O 205 205	0	0
2	B	232	Total O 232 232	0	0
2	C	132	Total O 132 132	0	0
2	D	39	Total O 39 39	0	0

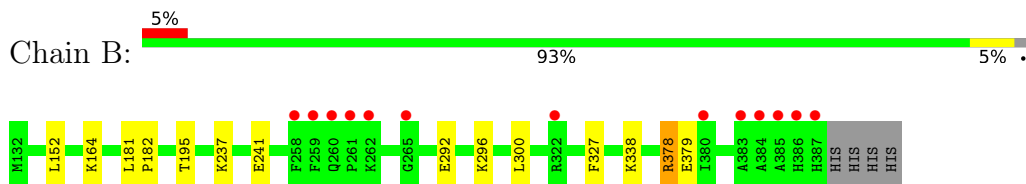
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

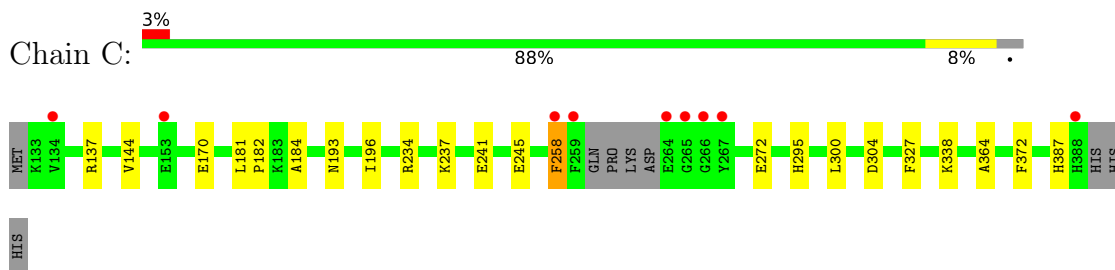
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



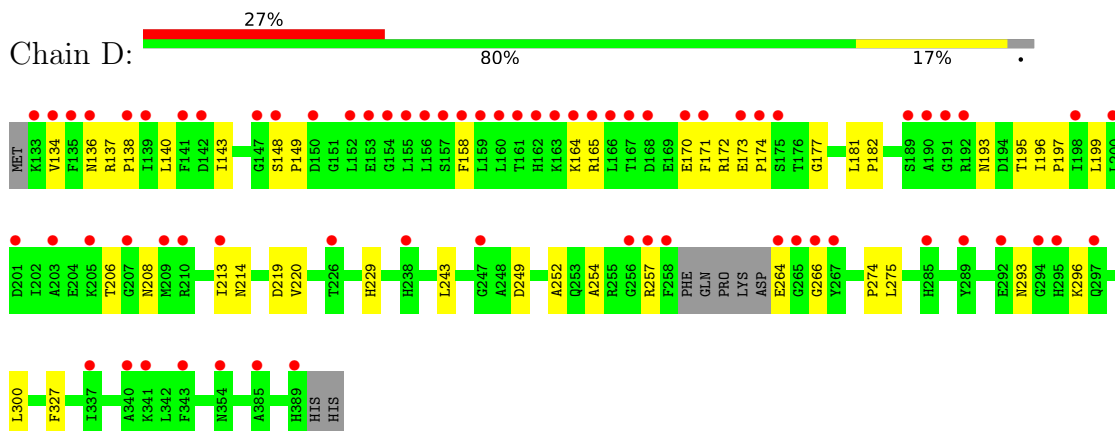
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.95Å 48.27Å 134.03Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	37.57 – 2.00 37.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.57-2.00) 99.7 (37.57-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.00Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.211 0.180 , 0.211	Depositor DCC
R_{free} test set	1821 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtrriage
Anisotropy	0.444	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8741	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0735e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/2138	0.58	1/2882 (0.0%)
1	B	0.47	0/2125	0.59	0/2866
1	C	0.35	0/2065	0.52	0/2786
1	D	0.31	0/2041	0.53	0/2754
All	All	0.40	0/8369	0.56	1/11288 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	2095	11	0
1	B	2058	0	2086	8	0
1	C	2009	0	2023	14	0
1	D	2001	0	2016	23	0
2	A	205	0	0	1	0
2	B	232	0	0	1	0
2	C	132	0	0	0	0
2	D	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8741	0	8220	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:NZ	1:A:241:GLU:OE2	2.26	0.69
1:D:164:LYS:NZ	1:D:170:GLU:OE2	2.25	0.67
1:B:237:LYS:NZ	1:B:241:GLU:OE2	2.30	0.64
1:A:300:LEU:HD11	1:A:338:LYS:HG2	1.81	0.61
1:C:237:LYS:NZ	1:C:241:GLU:OE2	2.34	0.60
1:D:275:LEU:HD21	1:D:300:LEU:HD23	1.84	0.59
1:D:213:ILE:HG23	1:D:243:LEU:HD22	1.86	0.58
1:B:292:GLU:OE1	1:B:338:LYS:NZ	2.36	0.58
1:D:140:LEU:HA	1:D:143:ILE:HD12	1.87	0.57
1:B:300:LEU:HD11	1:B:338:LYS:HG2	1.86	0.56
1:D:136:ASN:HA	1:D:171:PHE:HE1	1.71	0.56
1:C:258:PHE:H	1:C:258:PHE:HD2	1.53	0.55
1:D:165:ARG:NH1	1:D:206:THR:O	2.41	0.54
1:D:165:ARG:NH2	1:D:206:THR:O	2.43	0.52
1:A:292:GLU:OE1	1:A:338:LYS:NZ	2.44	0.51
1:B:152:LEU:HD11	1:B:195:THR:HB	1.93	0.51
1:C:300:LEU:HD11	1:C:338:LYS:HG2	1.92	0.51
1:D:165:ARG:NH1	1:D:208:ASN:HB2	2.27	0.50
1:A:245:GLU:HG2	1:A:295[A]:HIS:NE2	2.27	0.50
1:D:214:ASN:OD1	1:D:249:ASP:N	2.35	0.49
1:C:144:VAL:HG13	1:C:184:ALA:HB2	1.93	0.49
1:D:293:ASN:OD1	1:D:296:LYS:N	2.27	0.49
1:D:172:ARG:NH2	1:D:177:GLY:O	2.43	0.47
2:A:489:HOH:O	1:C:387:HIS:HD2	1.98	0.47
1:C:245:GLU:HG2	1:C:295:HIS:NE2	2.29	0.46
1:D:229:HIS:CE1	1:D:254:ALA:HB2	2.50	0.46
1:B:164:LYS:NZ	2:B:533:HOH:O	2.49	0.46
1:C:234:ARG:HA	1:C:234:ARG:HD3	1.74	0.46
1:C:258:PHE:CD2	1:C:258:PHE:N	2.84	0.46
1:C:364:ALA:HB2	1:C:372:PHE:CE1	2.52	0.45
1:A:145:SER:HB3	1:A:183:LYS:HE3	1.99	0.44
1:D:264:GLU:HG2	1:D:266:GLY:H	1.82	0.44
1:B:181:LEU:HB3	1:B:182:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:HA	1:D:174:PRO:HD3	1.85	0.43
1:D:196:ILE:HB	1:D:197:PRO:HD3	2.01	0.43
1:A:152:LEU:HD11	1:A:195:THR:HB	2.00	0.42
1:C:258:PHE:HD2	1:C:258:PHE:N	2.14	0.42
1:A:204:GLU:HA	1:A:209:MET:HB2	2.01	0.42
1:D:181:LEU:HB3	1:D:182:PRO:HD3	2.00	0.42
1:D:252:ALA:O	1:D:274:PRO:HD3	2.20	0.42
1:A:150:ASP:O	1:A:153:GLU:HG3	2.19	0.42
1:B:378[B]:ARG:NH1	1:B:379:GLU:OE2	2.47	0.42
1:D:137:ARG:HB3	1:D:138:PRO:HD3	2.00	0.42
1:D:134:VAL:HA	1:D:158:PHE:CE1	2.55	0.42
1:D:148:SER:HA	1:D:149:PRO:HD2	1.85	0.42
1:D:219:ASP:O	1:D:257:ARG:HD3	2.20	0.41
1:D:195:THR:O	1:D:199:LEU:HG	2.20	0.41
1:D:193:ASN:O	1:D:196:ILE:HG12	2.20	0.41
1:C:181:LEU:HB3	1:C:182:PRO:HD3	2.02	0.41
1:A:217:PHE:CZ	1:A:230:ILE:HD11	2.56	0.41
1:A:375:ILE:O	1:A:379:GLU:HG3	2.21	0.41
1:A:181:LEU:HB3	1:A:182:PRO:HD3	2.03	0.41
1:C:137:ARG:HB2	1:C:170:GLU:O	2.21	0.41
1:C:272:GLU:OE1	1:C:304:ASP:HB2	2.20	0.40
1:B:296:LYS:HE3	1:B:296:LYS:HB2	1.92	0.40
1:C:193:ASN:O	1:C:196:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/260 (100%)	254 (98%)	6 (2%)	0	100	100
1	B	259/260 (100%)	253 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	251/260 (96%)	245 (98%)	6 (2%)	0	100	100
1	D	248/260 (95%)	241 (97%)	7 (3%)	0	100	100
All	All	1018/1040 (98%)	993 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/221 (101%)	220 (99%)	3 (1%)	69	74
1	B	222/221 (100%)	219 (99%)	3 (1%)	67	72
1	C	216/221 (98%)	214 (99%)	2 (1%)	78	83
1	D	213/221 (96%)	211 (99%)	2 (1%)	78	83
All	All	874/884 (99%)	864 (99%)	10 (1%)	78	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	PHE
1	A	378[A]	ARG
1	A	378[B]	ARG
1	B	327	PHE
1	B	378[A]	ARG
1	B	378[B]	ARG
1	C	258	PHE
1	C	327	PHE
1	D	220	VAL
1	D	327	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/260 (98%)	-0.10	9 (3%) 44 43	16, 27, 68, 105	0
1	B	256/260 (98%)	-0.06	13 (5%) 28 27	15, 28, 70, 142	0
1	C	252/260 (96%)	-0.13	9 (3%) 42 42	29, 43, 65, 119	0
1	D	252/260 (96%)	1.23	69 (27%) 0 0	37, 84, 125, 186	0
All	All	1016/1040 (97%)	0.23	100 (9%) 7 7	15, 41, 108, 186	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	10.4
1	C	258	PHE	10.4
1	D	159	LEU	10.0
1	D	294	GLY	9.0
1	D	157	SER	8.6
1	C	266	GLY	8.6
1	D	171	PHE	8.1
1	B	261	PRO	7.4
1	D	139	ILE	6.8
1	C	265	GLY	6.7
1	D	135	PHE	6.6
1	D	265	GLY	6.3
1	A	261	PRO	6.1
1	D	266	GLY	6.1
1	B	260	GLN	6.1
1	D	258	PHE	6.0
1	D	170	GLU	5.9
1	D	207	GLY	5.9
1	D	163	LYS	5.8
1	A	262	LYS	5.7
1	D	138	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	160	LEU	5.6
1	D	292	GLU	4.8
1	D	155	LEU	4.8
1	D	238	HIS	4.8
1	D	210	ARG	4.6
1	B	384	ALA	4.4
1	D	136	ASN	4.4
1	D	340	ALA	4.3
1	B	262	LYS	4.3
1	D	166	LEU	4.3
1	D	389	HIS	4.2
1	D	156	LEU	4.2
1	C	134	VAL	4.2
1	D	190	ALA	4.1
1	C	259	PHE	4.0
1	D	154	GLY	3.8
1	D	341	LYS	3.5
1	B	265	GLY	3.5
1	D	152	LEU	3.5
1	D	297	GLN	3.3
1	D	257	ARG	3.3
1	C	267	TYR	3.2
1	D	205	LYS	3.1
1	D	203	ALA	3.1
1	D	168	ASP	3.1
1	D	226	THR	3.0
1	A	385	ALA	3.0
1	A	260	GLN	3.0
1	B	386	HIS	2.9
1	D	267	TYR	2.9
1	D	148	SER	2.9
1	D	200	LEU	2.9
1	D	247	GLY	2.9
1	D	165	ARG	2.9
1	D	158	PHE	2.8
1	D	192	ARG	2.8
1	D	175	SER	2.7
1	D	191	GLY	2.7
1	D	174	PRO	2.7
1	D	133	LYS	2.7
1	D	256	GLY	2.7
1	B	385	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	209	MET	2.6
1	A	265	GLY	2.6
1	D	164	LYS	2.5
1	B	387	HIS	2.5
1	D	198	ILE	2.5
1	A	386	HIS	2.5
1	D	189	SER	2.5
1	A	387	HIS	2.5
1	D	289	TYR	2.4
1	D	295	HIS	2.4
1	D	161	THR	2.4
1	D	201	ASP	2.4
1	D	173	GLU	2.3
1	B	258	PHE	2.3
1	D	264	GLU	2.3
1	A	132	MET	2.3
1	D	162	HIS	2.3
1	D	285	HIS	2.3
1	D	343	PHE	2.2
1	B	380	ILE	2.2
1	D	150	ASP	2.2
1	C	153	GLU	2.2
1	D	147	GLY	2.2
1	D	153	GLU	2.2
1	D	167	THR	2.2
1	B	383	ALA	2.2
1	D	141	PHE	2.1
1	D	354	ASN	2.1
1	C	264	GLU	2.1
1	C	388	HIS	2.1
1	B	259	PHE	2.1
1	D	385	ALA	2.1
1	D	337	ILE	2.1
1	D	213	ILE	2.0
1	A	382	ASP	2.0
1	D	142	ASP	2.0
1	B	322	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.